
Accuracy of Differential Sensitivity for One-Dimensional Shock Problems

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Outline

- *Motivation*
- *Sensitivity methods*
 - *Compatible operators for DST*
- *1D Example problems*
 - *Convergence study*
- *Conclusions*

The Analysis Exercise



$$\vec{\gamma} = (\gamma_1, \gamma_2, \dots, \gamma_N)^T \quad \vec{R} = (R_1, R_2, \dots, R_M)^T$$

Would like to know:

1. *What is the sensitivity of an output Response to the input?*
2. *To which parameters is the response most sensitive?*
3. *What is the uncertainty of an output Response to input uncertainties?*
4. *How can the input be tuned to obtain an optimum output Response?*

The Sensitivity

- ***The sensitivity ($\frac{\vec{R}}{\vec{x}}$) can help the analysis process***
- ***How is the sensitivity obtained?***
 - Direct Method - [1]
 - Forward Differential Sensitivity Theory (DST), numerical solution of differentiated PDEs - [2]
 - Forward Differential Sensitivity Analysis (DSA), differentiated difference equations - [3]
 - Adjoint DST, numerical solution of adjoint PDEs - [4]
 - Adjoint DSA, transpose of DSA equations - [5]
 - Automatic Differentiation (AD) - [6]
 - Adjoint Differentiation In Code Technique (ADICT)- [7]

DST Method - Mathematical Technique

$$N[\bar{y}(\bar{x}), \cdot] = O(\bar{x}, \cdot) \quad (1)$$

$$R = \int_{t_0}^{t_f} F(\bar{y}, \bar{x}) d\bar{r} dt \quad \langle F(\bar{y}, \bar{x}) \rangle \quad (2)$$

— (Eq. 1) $L \frac{\bar{y}}{\bar{y}} = \bar{s}$ (3) **Basis of Forward DST**

— (Eq. 2) $\frac{R}{t_f - t_0} = \frac{\bar{F}}{\bar{y}} \cdot \frac{\bar{y}}{d\bar{r} dt} \quad \left\langle \frac{\bar{F}}{\bar{y}}, \frac{\bar{y}}{d\bar{r} dt} \right\rangle \quad (4) \quad \text{Sensitivity}$

Inner product math:

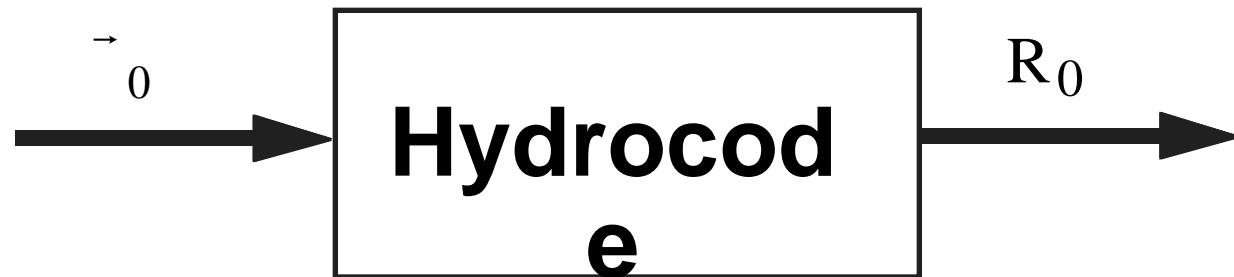
defines adjoint Eqs. $L^* \bar{y}^* = \bar{s}^*$ (5)

& produces sensitivity

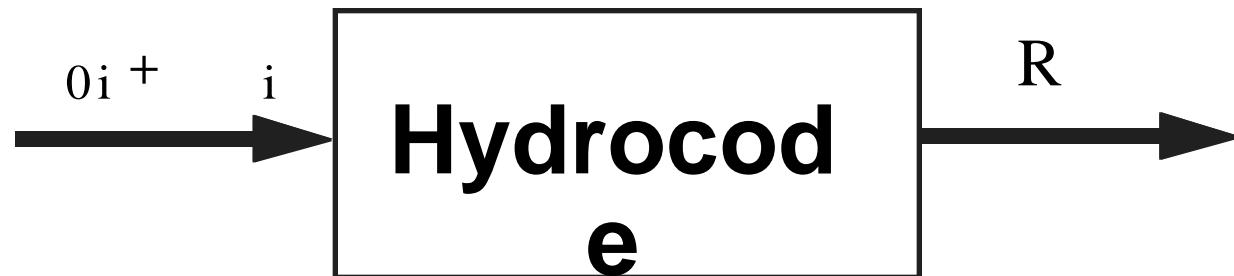
$$\frac{R}{t_f - t_0} = \left\langle \bar{s}, \bar{y}^* \right\rangle - B \left\langle \bar{y}, \bar{y}^* \right\rangle \quad (6) \quad \text{Basis of Adjoint DST}$$

[1] Direct Method

Perform the base case calculation:

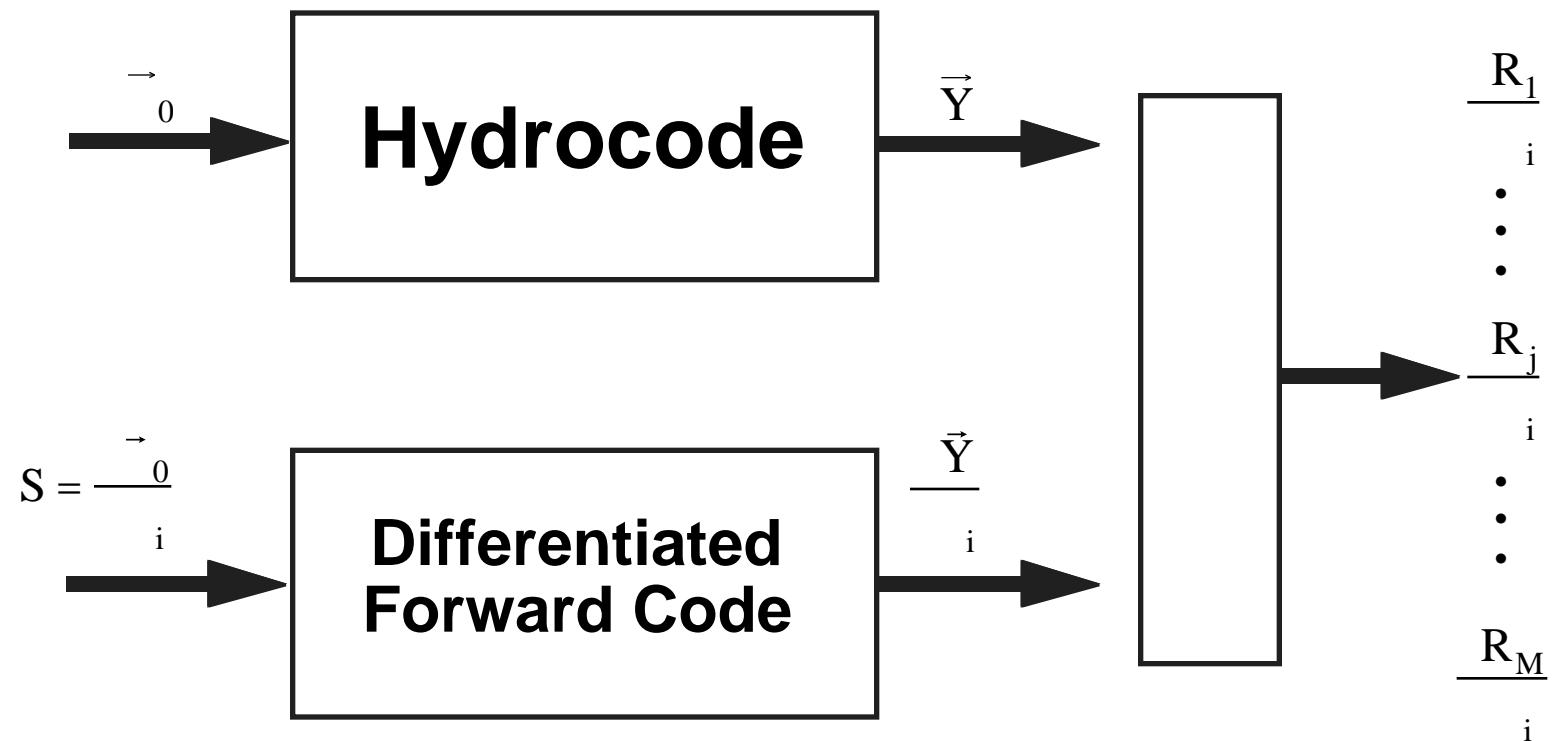


Repeat "N" times:



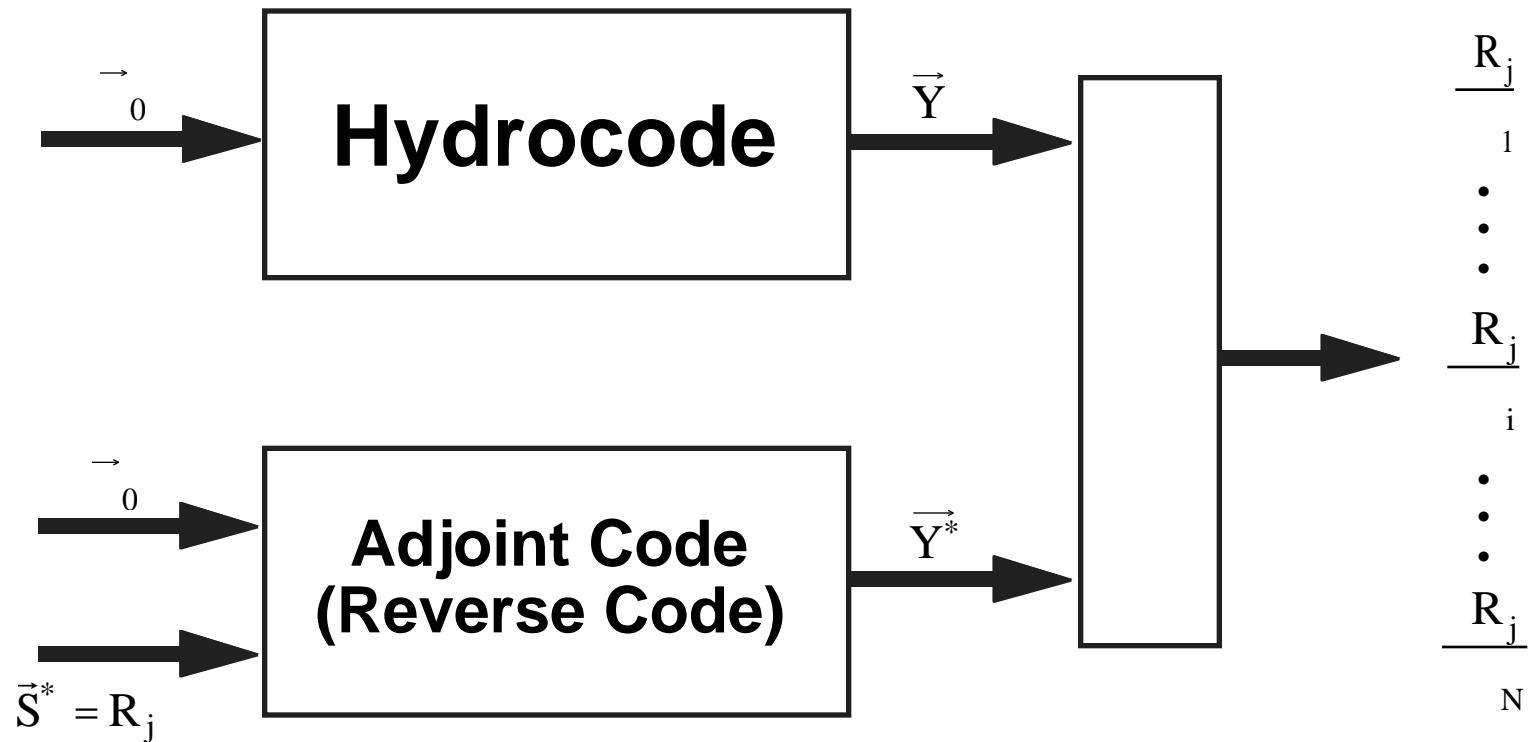
Approximate with finite differences: $\frac{R}{i} \quad \frac{(R - R_0)}{i}$

[2 & 3] Forward DST/DSA Method



Forward methods most efficient for one parameter with many responses

[4 & 5] Adjoint DST/DSA Method



Adjoint methods most efficient for one response with many parameters

1D Adjoint DST Equations

$$\vec{y}^* = \begin{pmatrix} *, & *, & *, & * \\ , & z, & , & \end{pmatrix}^T$$

$$-\frac{D}{Dt} \frac{*}{z} + \frac{Du_z}{Dt} - g \frac{*}{z} + \frac{Di}{Dt} I^* - \frac{P}{z} = \frac{F}{u_z}$$

$$-\frac{*}{z} - \frac{D}{Dt} \frac{*}{z} + \frac{u_z}{z} - P \frac{I^*}{z} - \frac{P}{z} I^* + \frac{i}{z} I^* + \frac{q}{z} + q \frac{*}{z} = \frac{F}{u_z}$$

$$-\frac{DI^*}{Dt} - \frac{P}{i} = \frac{F}{i}$$

$$* - \frac{*}{z} + \frac{u_z}{z} I^* = \frac{F}{P}$$

Method of Support Operators [Shashkov]:

Finding difference operators for the adjoint DST equations

$$\text{Inner product} \quad \int_V s q (\cdot \cdot \vec{v}) dV = - \int_V q \vec{v} \cdot s dV - \int_V s \vec{v} \cdot q dV + \int_S s q (\vec{v} \cdot d\vec{S})$$

Example: * in adjoint momentum Eq.

$$\int_V^* (\cdot \cdot \vec{v}) dV = - \int_V^* (\cdot \cdot \vec{v}) dV \quad \int_0^L \frac{*z}{z} dz = - \int_0^L \frac{*z}{z} dz - \int_0^L \frac{*z}{z} dz$$

Finite difference form

$$\sum_j j \cdot j^* \text{DIV}(\cdot z)_j = - \sum_j z,j \cdot j \text{GRAD}(\cdot)_j^* - \sum_j z,j \cdot j^* \text{GRAD}(\cdot)_j$$

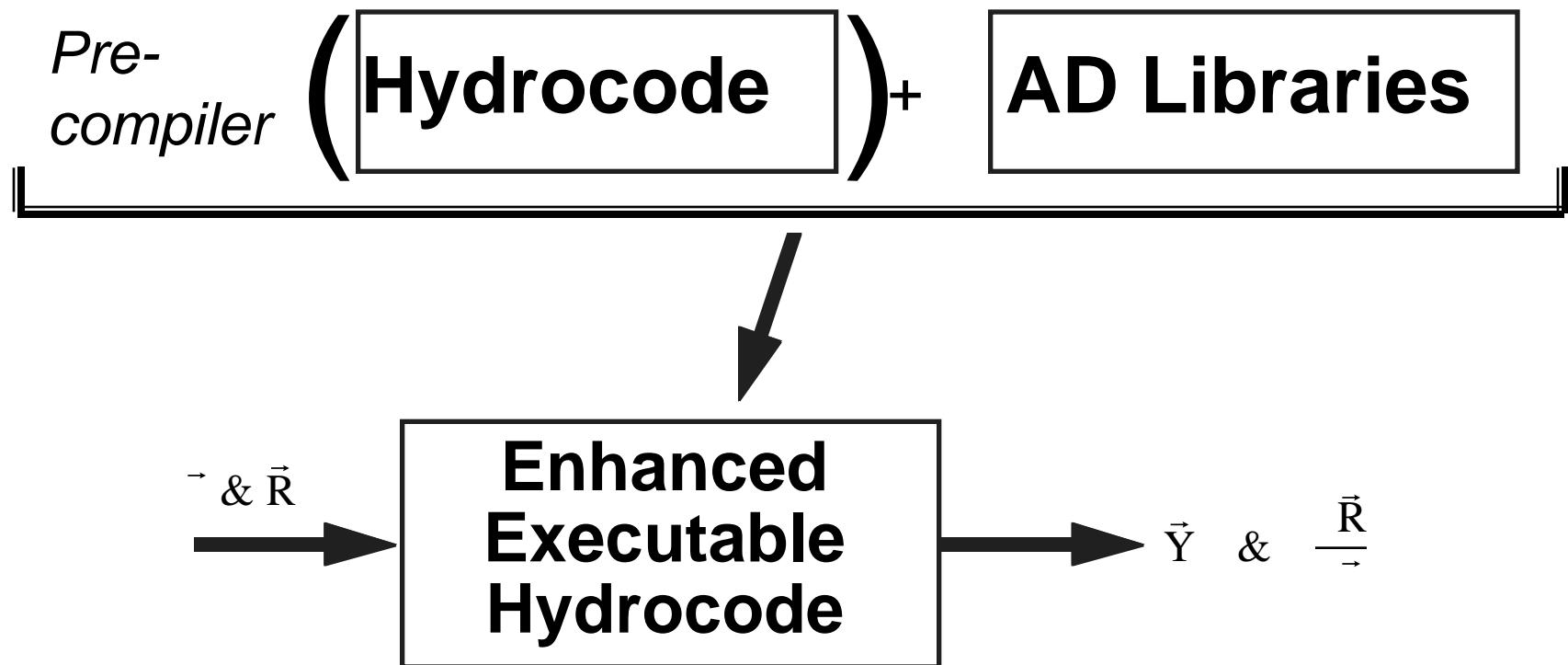
Solve for $[\text{GRAD}(\cdot)]_{j+\frac{1}{2}}$

$$[\text{GRAD}(\cdot)]_{j+\frac{1}{2}} = \frac{j+1^* - j^*}{z} - \frac{1}{2} \cdot j^* \frac{j - j-1}{z} + j+1^* \frac{j+1 - j}{z}$$

Adjoint DSA - DST Equivalence

- *Support operator [Shashkov] generated adjoint DST difference equations and Tranposed forward DSA difference equations result in the same adjoint difference equations for simple numerics*
- *Method of support operators not demonstrated for MESA-like numerics*

[6] Automatic Differentiation (AD) Method



Worked well for simple 1D code, impractical for “real” code

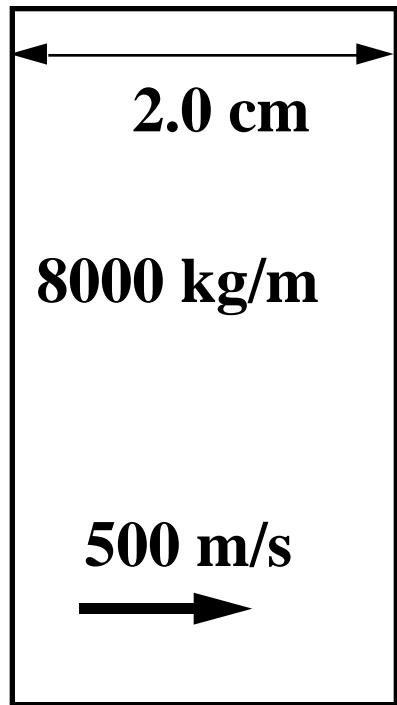
[7] ADICT Method

- Change original Hydrocode to be top-down, in-line, break into logical blocks
- Manually code adjoint, beginning with Response (reverse chain rule, solved backwards in time) -Forward solution must be available as with DST & DSA
- AD may be used to produce differentiated code



Worked well for simple 1D code, being applied to 1D CHARADE code

1D Metal Flow Problem Specifications



Parameters

$$(t = 0) = 8000 \text{ kg} / \text{m}^3$$

$$u_z(t = 0) = 500 \text{ m} / \text{s}$$

$$c_0 = 4000 \text{ m} / \text{s}$$

$$\rho_0 = 8000 \text{ kg} / \text{m}^3$$

$$s = 1.0$$

$$= 0.0$$

$$c_L = 0.2$$

$$c_Q = 2.0$$

$$u_z(z = L) = 400 \text{ m} / \text{s}$$

$$(z = 0) = 8000 \text{ kg} / \text{m}^3$$

$$u_z(z = 0) = 500 \text{ m} / \text{s}$$

Response

$$R = \int_{t_z}^{t_f} P(z) \frac{1}{L t_f} dz dt = \bar{P}$$

Adjoint Source

$$\frac{\vec{F}}{\vec{y}} = (0, 0, 0, 1/L t_f)^T$$

1D, 1 Mat'l Flow Problem Results-1

Sensitivity	ADIFOR	ADICT	% ERROR	DSA Forward	% ERROR
$\bar{P}/(t = 0)$	1.592504E+07	1.592504E+07	0.00000	1.592504E+07	-0.00003
$\bar{P}/u_z(t = 0)$	1.462557E+05	1.462583E+05	-0.00178	1.462543E+05	0.00097
\bar{P}/c_0	1.538857E+05	1.538856E+05	0.00006	1.538880E+05	-0.00151
$\bar{P}/_0$	-1.607631E+07	-1.607631E+07	0.00000	-1.607632E+07	-0.00006
\bar{P}/s	1.017310E+07	1.017310E+07	0.00005	1.017290E+07	0.00193
$\bar{P}/$	-2.494427E+06	-2.494427E+06	0.00000	-2.494382E+06	0.00181
\bar{P}/c_L	7.984238E+04	7.984239E+04	-0.00001	7.984247E+04	-0.00012
\bar{P}/c_Q	4.221503E+06	4.221508E+06	-0.00012	4.221503E+06	-0.00001
$\bar{P}/u_z(z = L)$	-4.009899E+06	-4.009902E+06	-0.00007	-4.009900E+06	-0.00002
$\bar{P}/(z = 0)$	1.990000E+05	1.990001E+05	-0.00005	1.990003E+05	-0.00017
$\bar{P}/u_z(z = 0)$	3.824008E+06	3.824007E+06	0.00003	3.824011E+06	-0.00007

$$\bar{P} = 0.38179514 \text{ GPa}$$

ADIFOR provides the "correct" sensitivity for comparison

1D, 1 Mat'l Flow Problem Results-2

Sensitivity	ADIFOR*	Adjoint DSA/DST	% ERROR	MESA2D DST	% ERROR
$\bar{P}/(t = 0)$	1.592504E+07	1.592505E+07	-0.00003	1.592474E+07	0.00190
$\bar{P}/u_z(t = 0)$	1.462557E+05	1.457602E+05	0.33880	1.437188E+05	1.73454
\bar{P}/c_0	1.538857E+05	1.538705E+05	0.00986	1.532389E+05	0.42034
$\bar{P}/_0$	-1.607631E+07	-1.607631E+07	-0.00001	-1.595601E+07	0.74832
\bar{P}/s	1.017310E+07	1.017203E+07	0.01051	9.987033E+06	1.82901
$\bar{P}/$	-2.494427E+06	-2.494166E+06	0.01048	-2.449330E+06	1.80790
\bar{P}/c_L	7.984238E+04	7.983290E+04	0.01187	7.928956E+04	0.69238
\bar{P}/c_Q	4.221503E+06	4.220765E+06	0.01747	4.118080E+06	2.44990
$\bar{P}/u_z(z = L)$	-4.009899E+06	-4.025325E+06	-0.38470	-3.970886E+06	0.97291
$\bar{P}/(z = 0)$	1.990000E+05	2.010004E+05	-1.00521	1.980054E+05	0.49980
$\bar{P}/u_z(z = 0)$	3.824008E+06	3.856009E+06	-0.83685	3.803290E+06	0.54180

$\bar{P} = 0.38179514$ GPa

* ADIFOR provides the "correct" sensitivity for comparison

1D, 1 Mat'l Problem Convergence Study

- *DST, which is based on a simplified numerical scheme, requires that the physical solution is converged*
- *When comparing the MESA solution to the simple forward solution (basis of DST) we found that the rate of convergence is different*
- *Effects on sensitivity are substantial*

Summary

- *Provided description of sensitivity techniques*
- *Showed that DST & DSA can be made equivalent when using compatible difference operators for DST*
- *Successfully applied AD techniques for test case*
- *Introduced ADICT, which is being applied to a “real” hydrocode*
- *Demonstrated accurate sensitivities for a 1D problem*
- *Goal is to provide a package of practical methods that can be used for design purposes*

Conclusions

- *Early DST applications which used simple difference operators provided accurate sensitivities because physical solutions were converged*
- *DST requires either compatible operators or a converged physical solution*
- *MESA and Current DST difference operators are not compatible*
- *AD techniques impractical for real hydrocode applications*
- *Accurate sensitivities for arbitrary resolution require a code-based approach (**AD, DSA, ADICT**)*